Q Resolution on LOQ at ISIS

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The resolution on LOQ has been estimated numerically for situations typical of normal operations. Since any one Q value on LOQ is obtained from a range of different wavelengths and detector radii the resolution function should be an appropriately weighted average of Gaussian terms. This average is reasonably well described by a Gaussian in the peak though, except at the extremes of Q, it has broader tails. To date detailed results are available for an 8mm sample diameter and incident wavelengths of 2.2-10 Å or 6-10 Å. Initial results have also been produced for the new high angle bank (HAB) with 2-10 Å neutrons, for which the resolution averages begin to show some asymmetry to higher Q. This asymmetry is introduced by allowing for the likely time distributions of neutrons of a given wavelength. Estimates have been made of the effect of increasing the diameter of the sample aperture. Some FORTAN routines which compute the necessary parameters are available from the author (or may be found in the GENIE function LOQ$DISK0:[LOQMGR]RESOL_CALC.FOR).

Method of calculation

The numerical summations used mimic the normal methods of combining data in COLETTE for scalar Q. An incident spectrum shape recorded on the LOQ ORDELA detector is used. Simultaneous summation of a "time-of-flight" spectrum for given scattering laws produced results in close, absolute, agreement with those actually seen on the instrument. The new estimated resolution function is worse at low Q and better at high Q than a 1988 estimate, which considered the BF_3 LETI detector (see Figure 1).

The basic resolution equation, for the standard deviation of scalar Q, σ_Q, from Mildner & Carpenter [1] is :

$$(\sigma_Q)^2 = \frac{1}{12}\left(\frac{2\pi}{\lambda}\right)^2\left[3\frac{R_1^2}{L_1^2} + 3\frac{R_2^2}{L'^2} + \frac{(\Delta R)^2}{L_2^2} + \frac{R^2}{L_2^2}\left(\frac{\Delta\lambda}{\lambda}\right)^2\right] \tag{1}$$

Where beam defining apertures of radii R_1 and R_2 are separated by L_1 , and we assume that the small angle approximation is valid so that $Q = 2\pi\theta/\lambda = 2\pi R/\lambda L_2$, where R is a radius on the detector at distance L_2 from the sample. Allowing for a distance L_X between the second aperture and the sample, and for

$$\frac{1}{L'} = \frac{1}{L_1} + \frac{1}{L_2}$$

one obtains

$$\left(\frac{\sigma_Q}{Q}\right)^2 = \left(\frac{R_1(L_X + L_2)}{2RL_1}\right)^2 + \left(\frac{R_2(L_1 + L_X + L_2)}{2RL_1}\right)^2 + \frac{1}{12}\left(\frac{\Delta R}{R}\right)^2 + \frac{1}{12}\left(\frac{\Delta\lambda}{\lambda}\right)^2 \tag{2}$$

where ΔR and $\Delta\lambda$ are rectangular bin widths for the detector radius and wavelength step selected. The standard deviation of a rectangular distribution of width Δ is $\Delta/\sqrt{12} = \Delta/3.4641$

Note that resolution σ_Q is only parallel to Q, the component perpendicular to Q has been neglected, see for example Pedersen et.al. [2]. At small Q this may become significantly large, at higher Q it should be neglible. [RKH needs to investigate further] In any case there may also be effects at small Q due to the beam stop, so the resolution functions proposed here should be treated only as approximate at small Q to avoid over-interpretation of data.

Instrumental parameters for LOQ

We need to decide values for the effective detector resolution ΔR and wavelength resolution $\Delta\lambda$ for LOQ. The wavelength term is a convolution of the bin width used in the data reduction procedure, normally 0.05 Å with a term due to the intrinsic time spread of any given wavelength produced by the ISIS hydrogen moderator. Data are collected in time bins of $\Delta t/t$ = 2.5% at both the incident beam monitor and the main detector. This imposes a further limitation, as discussed below.

(i) Wavelength resolution

Neutrons of a given wavelength are distributed in time with a relatively sharp leading edge and then an exponentially decaying tail [3]. For the ISIS hydrogen moderator the time constant of the tail should increase from about 40 μsec at 2 Å to saturate at about 100 μsec around 5.5 Å. As far as resolution is concerned the standard deviation of the pulse shape is very close to the exponential time constant. More detailed calculations, described below, allow for a more realistic, asymmetric, pulse shape.

For a neutron wavelength of 10 Å we predict using t (μsec) = 252.7 D (m) λ(Å) that the equivalent rectangular pulse width is Δt = 366.5 μsec, leading to $\Delta\lambda$ = 0.097 Å at distance D =10 m, (around the monitor position) or $\Delta\lambda$ = 0.145 Å at D = 15 m (the main detector).

Similarly for a 2 Å neutron Δt = 147.2 μsec, leading to $\Delta\lambda$ = 0.058 Å at D = 10m or 0.039 Å at D = 15 m. Since all data on LOQ is rebinned to match the monitor spectrum, the resolution there should perhaps be the most appropriate to use. It should be mentioned here that LOQ collects data in bins of $\Delta t/t$ = 2.5%, which was based on an early report of a 150 μsec decay tail, as well as practical limitations on data file size. In view of this more recent information it seems that time channels at long wavelength would be better matched at 1 - 1.5 %. With new data compression routines soon to be available a change should be possible, though since the geometry terms dominate the resolution at small Q it will not make any practical difference.

Taking the most conservative view, convoluting $\Delta\lambda$ with $\Delta t/t$ = 2.5%; the wavelength resolution $\Delta\lambda/\lambda$ on LOQ is effectively 3.8% at 2Å and 2.9% at 10 Å, compared to typically 10% FWHM (= 14.7 % $\Delta\lambda/\lambda$), or more , on reactor sources.

(ii) Detector resolution

Spatial resolution of the main ^{3}He detector has been estimated using data collected with a cadmium mask with 121 holes, mostly of 20mm diameter, that may be placed in front of the detector. The mask is primarily used to calibrate the non-linear position response of the detector at its edges. A fitting program, CDFIT, convolutes a two dimensional Gaussian resolution function with each hole in a least squares fit of both position and resolution. By rotating the mask through four successive orientations the 64 cm x 64 cm detector may be surveyed on a 3 cm grid. Detector resolution σ_D averages to 5.6 mm, with most values around 5-6 mm and a few from 3.5 to 7.5, though these latter may be more due to poor counting statistics at the edges of the detector. (Some older data, from before the Sept. 95 refurbishment of the detector gave σ_D = 4.6 mm. A slightly relaxed resolution should enhance the detector lifetime.)

The detector "pixels" are generated electronically as a function of the pulse rise time encoding used. The effective pixel size is presently 2 x 5.267 = 10.534 mm for 64 x 64 pixels. COLETTE groups pixels, by the radius of their centre points, into "rings" of width 6 mm. Convoluting these two quantities together, we might expect σ = 3.50 mm [= $((10.53^2 + 6^2)/12)^{1/2}$]. Numerical calculations summing some actual distributions in 0.25mm steps, are fit by Gaussians of σ_{RING} = 3.80 mm, though the actual distribution falls off faster in the wings. Taking the latter value and convoluting with the measured σ_D= 5.6 mm we obtain σ_R = 6.77 mm, equivalent to a rectangular distribution of ΔR = 23.44 mm. For 128 x 128 pixels σ_{RING} improves to 2.5 mm, but since σ_D

dominates, ΔR only reduces to 21.24 mm. Hence there is little intrinsic advantage in routinely operating with 128 x 128 pixels.

The high angle bank uses 12 mm square pixels of scintillator, which are actually four sub-pixels of 6 mm permanently linked together. Thus we simply convolute 12 mm with the 6 mm ring width to obtain ΔR = 13.5 mm. Ultimately we may have to look for "edge effects" between adjacent pixels or sub-pixels.

Inclusion of neutron pulse shapes

The resolution function in equation (2) is summed numerically, by program RESQ_AVG, in a way that closely mimics the actual data reduction process used in COLETTE for an isotropic scatterer. To obtain more realistic results for the $\Delta\lambda$ term an asymmetric neutron pulse shape distribution for each wavelength bin contributing to a particular value Q may be directly convoluted with a symmetrical Gaussian representing the remaining terms in (2).

The neutron pulse shape at any wavelength has essentially a sharp leading edge, approximated by a Gaussian, which is followed by a much longer exponential tail. A separate paper describes and discusses the pulse shapes in more detail, see also reference [3].

The time constant of the tail is of order 40 μsec at 2 Å, increasing linearly with wavelength to a maximum of about 100 μsec above 5 Å. Compared to arrival times of neutrons at the LOQ detectors of from 6.4 msec, for 2.2 Å at the HAB, up to 38.2 msec for 10 Å at the main detector the widths of the distributions are of only minor effect. On LOQ this effect only becomes noticeable for the HAB detector, since for shorter time of flight the time spread of the tail is more significant, and Q varies faster with wavelength at short wavelengths. (For proposed new cold neutron sources, with a "coupled" moderator, the tails might be three times longer and hence of more significance.)

A precise description of Q resolution also requires a precise definition of scattering variable Q, as discussed in the next section. Here is is assumed that a notional wavelength λ corresponds to the mean of its time distribution. (If one were considering a Bragg scatterer, then due to the sharp leading edge, one might assign effective wavelengths closer to the peak.)

The Q and wavelength loops in RESQ_AVG define $Q_0 = (4\pi/\lambda_0)\sin(\theta/2)$ for a particular wavelength (i.e. time) bin centred on λ_0 and a particular radial bin on a detector. For values Q' of the Q space resolution curve of that bin we compute only the component of resolution due to the pulse shape. If other wavelengths λ' arrive at the same time as wavelength λ_0 then they correspond to scattering at $Q' = (4\pi/\lambda')\sin(\theta/2)$ where $\lambda' = \lambda_0 Q_0/Q'$.

If wavelength λ_0 originates in the moderator pulse shape $N(\lambda_0, t)dt$ at a time t_0, assumed to be the mean time of $N(\lambda_0,t)$, then for a detector at distance D (metres), the arrival time in μsec is:

$cD\lambda' + t' = cD\lambda_0 + t_0$ where conversion factor c = 252.78,

If the start time of neutrons of wavelength λ', t', is greater than zero and neutrons λ' would, at least approximately, pass through the wavelength selecting chopper, then the pulse shape component of the resolution at $Q = Q'$ is given by $N(\lambda', t')\Delta t'$ where $\Delta t'$ is the width of the time slice around λ' corresponding to the Q' bin size $\Delta Q'$. It may be shown that:

$\Delta t' = cD\lambda'\Delta Q'/ Q'$

The resultant asymmetric resolution curve, already in Q space, is then numerically convoluted with a symmetrical Gaussian for the rest of the resolution function, including the terms for geometry and wavelength bin size. The resolution curves are considerably over-sampled at steps of $\Delta Q'/Q' = 10^{-3}$, and are only rebinned to a workable size before being written to file.

Empirical resolution functions

Calculated resolution peaks from RESQ_AVG for a series of points Q_0 were fit by least squares. A number of different models were tried to simulate the broadened tails of the Gaussian. A Voigt function (a Gaussian convoluted with a Lorentzian) was not suitable. A "stretched Gaussian" proved both effective and computationally simple:

$$G(x) \propto \exp\left\{-\frac{1}{2}\left(\frac{x}{\sigma_1 + \sigma_2|x| + \sigma_3 x}\right)^2\right\} \qquad \text{where } x = Q - Q_0 \qquad (3)$$

Parameter σ_2 symmetrically broadens the tails of the Gaussian generated by σ_1. Parameter σ_3 is used when needed to introduce asymmetry. For each instrumental configuration parameters σ_i were plotted against Q_0 and then fitted to simple functional forms, as shown in the Figures 1-3, and available in FORTRAN routines. To allow a certain amount of extrapolation, and to minimise spurious oscillations, some of the empirical fits have different functional forms for different parts of the Q range, so may exhibit some minor discontinuities. To match previous FWHM($\delta Q/Q$) plots σ_1 is shown as $2.35482\sigma_1/Q$. When $\sigma_2 = \sigma_3 = 0$ then σ_1 is the standard deviation and FWHM = $(8\log_e(2))^{1/2}\sigma_1$. Future plans are to attempt to automatically fit and tabulate the predicted resolution function at more values of Q, as generating the empirical parametrisation of the σ_i here requires a great deal of effort.

Samples larger than 8mm diameter.

The effect of increasing the diameter of the beam defining aperture before the sample has been estimated by noting the increase of the mean FWHM (assuming a symmetrical pulse shape) compared to the standard 8mm aperture. The increase is roughly linear with Q, the more so for the HAB, with the worst effect at small Q. The σ_I of equation (3) should be multiplied by the factors in the tables below for the diameter and Q range of interest.

LOQ main detector 2.2 - 10 Å, estimated increase of σ_i over A2 = 8 mm			
	A2 = 10 mm	A2 = 12 mm	A2 = 14 mm
low Q	1.045	1.105	1.17
high Q	1.035	1.085	1.14

LOQ HAB 2.2 - 10 Å, estimated increase of σ_i over A2 = 8 mm			
	A2 = 10 mm	A2 = 12 mm	A2 = 14 mm
low Q	1.060	1.13	1.21
high Q	1.035	1.08	1.13

Other minor effects ?

Not yet allowed for on LOQ, due to lack of experimental information, is the variation in mean emission time of neutrons from the moderator. This is a further effect of the asymmetric neutron pulse shape, in addition to its effect on Q space resolution discussed above. On LOQ the difference in mean emission time between 2 and 10 Å could be around 100 μsec. Thus if our time to wavelength conversion is perfectly correct at 10 Å, a shift of 100 μsec would, at distance D = 10m be an error of 0.04 Å at 2 Å, with perhaps a 1 to 2% error in the derived Q. Conversely if our time to wavelength conversion is correct at 2 Å, we have only a 0.4% error in Q at low Q.

The resolution calculations above assumed that the time to wavelength conversion was properly "focussed" to the mean emission time at each wavelength, something which COLETTE does not yet do. Ignoring this has only an insignificant effect on the shape of the LOQ resolution functions. (The effect of the mean emission time correction becomes more important at short time or distance, and short wavelength, especially for the longer tails from the "coupled" moderators proposed for future sources.)

We might also consider how well we know detector distances which should be correct to fractions of a percent. The ORDELA detector has a 4.4 cm thick, gas filled, detection region. This in itself gives an additional uncetainty in time or wavelength Δt of 22.2 μsec at 2 Å or 111.2 μsec at 10 Å, thus the $\Delta\lambda$ values given above should have been increased slightly. (From 147.2 to 148.9 μsec at 2Å, or from 366.5 to perhaps 383.0 μsec at 10 Å, though it is likely that the longer wavelengths are stopped in a shorter time than this.)

For the high angle bank it will be important to measure its position both absolutely and relative to the sample. We should investigate whether a Be filter will enable us to do this. Other beam lines calibrate their distances with neutron absorption resonances below $\lambda = 1$ Å which are not accessible on LOQ due to its bender.

References

[1] D.F.R.Mildner & J.M.Carpenter, J.Appl.Cryst. 17(1984)249-256.

[2] J.S.Pedersen, D.Posselt & K.Mortensen, J.Appl.Cryst.23(1990)321-333.

[3] Y.Kiyanagi, N.Watanabe, M.Furusaka, H.Iwasa & I.Fujikawa, ICANS XI (1990) 388-400, KEK Report 90-25.

Figure Captions

Note - Q ranges of data shown in these figures are slightly greater than normally available on LOQ. An asymmetric neutron pulse shape was used to estimate σ_1 , σ_2 and σ_3 for equation (3).

1. LOQ main detector, λ = 2.2 - 10 Å. Mean FWHM (symmetric neutron pulse) - line; $2.35\sigma_1/Q$ - line with +++ ; σ_2 - line with circles; previous FWHM estimate for LETI detector - triangles.

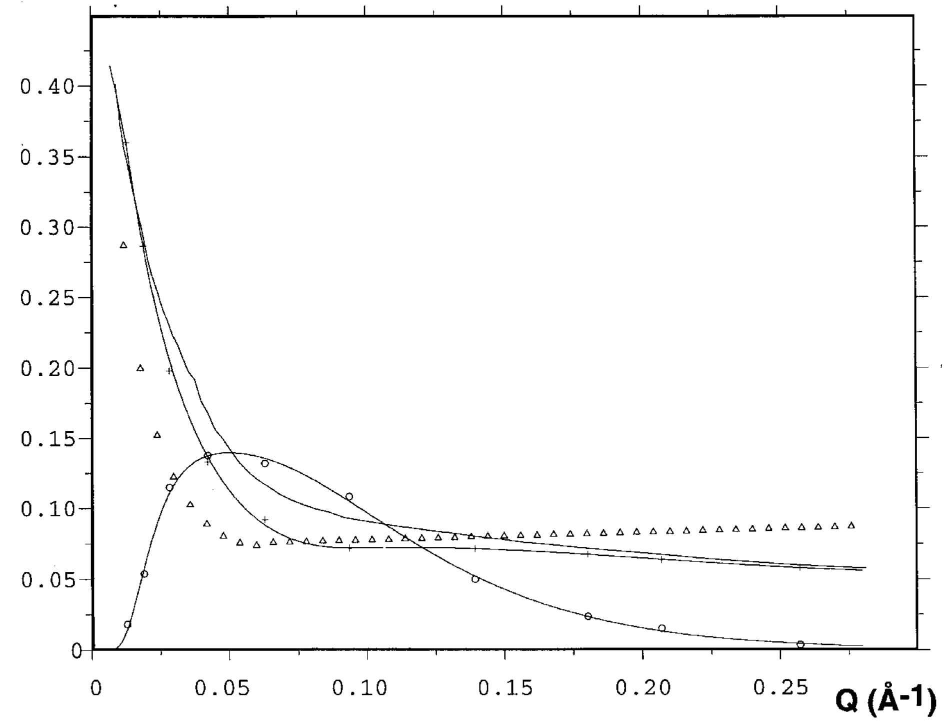
2. LOQ main detector, λ = 6 - 10 Å. Mean FWHM (symmetric neutron pulse) - line; $2.35\sigma_1/Q$ - line with +++ ; σ_2 - line with circles; mean FWHM for 2.2 - 10 Å, as Figure 1 - triangles. .

3. LOQ HAB, high angle bank, λ = 2 - 10 Å. . Mean FWHM (symmetric neutron pulse) - line; $2.35\sigma_1/Q$ - line with +++; σ_2 - line with circles; σ_3 - line with squares; mean FWHM for 2.2 - 10 Å, as Figure 1 - triangles.

RESOL_1.DOC

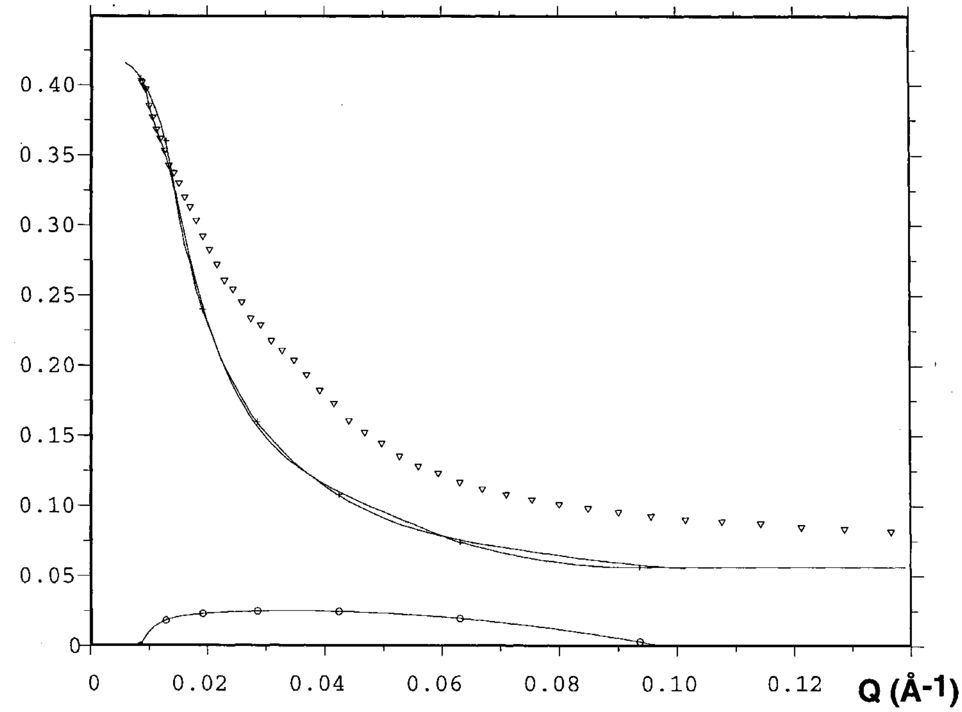
30/4/96
LOQ 2-10
mean FWHM —
2.35σ/Q ++
σ_2 —
(ΔΔ LETI)

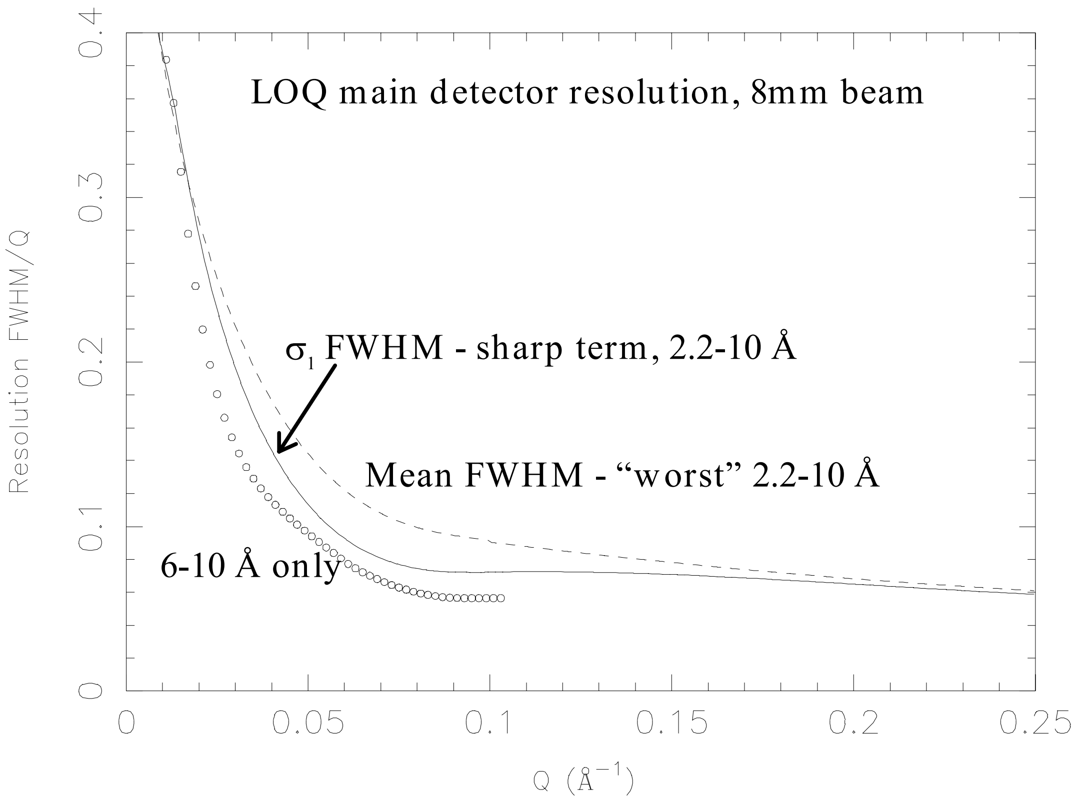
Fig. 1

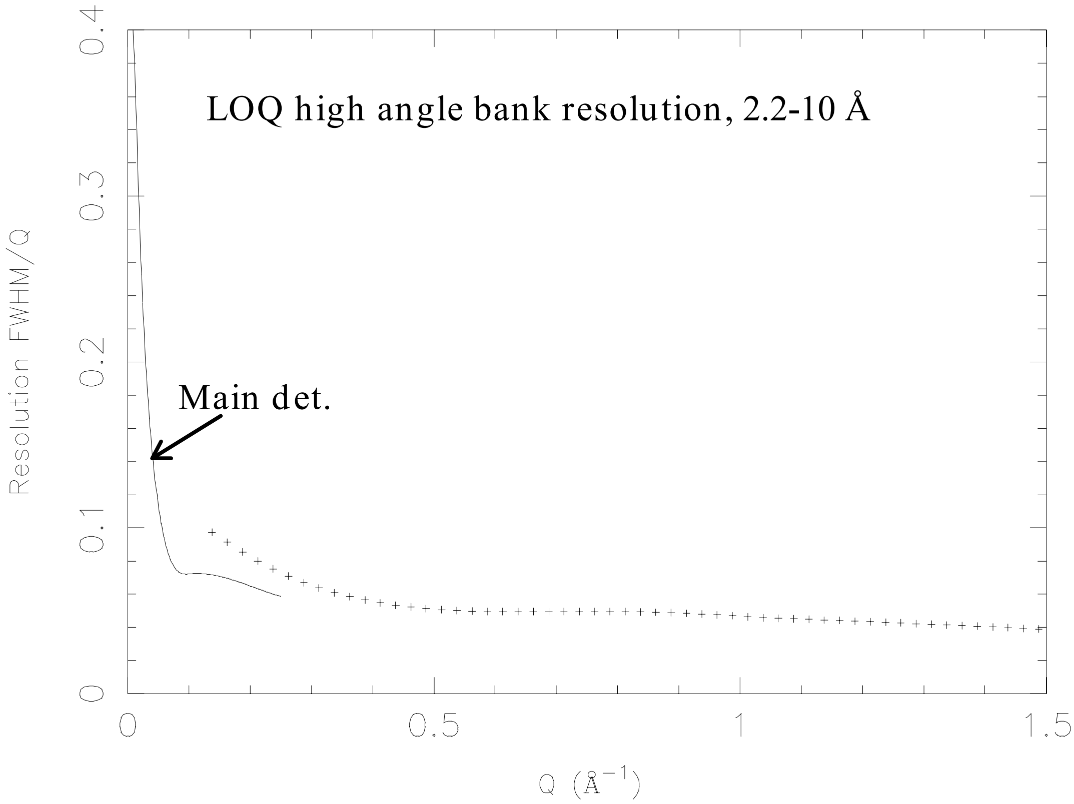


30/4/96
LOQ 6-10
(∇∇ 2-10)
2.35σ/Q
mean FWHM }
σ_2 ○○○

Fig. 2




LOQ main detector resolution, 8mm beam
σ1 FWHM - sharp term, 2.2-10 Å
Mean FWHM - "worst" 2.2-10 Å
6-10 Å only
Resolution FWHM/Q
Q (Å^{-1})
0
0.1
0.2
0.3
0.4
0.05
0.15
0.25


LOQ high angle bank resolution, 2.2-10 Å
Main det.
Resolution FWHM/Q
Q (Å^{-1})
0
0.1
0.2
0.3
0.4
0.5
1
1.5